

High resolution wavenumber standards for the infrared. (IUPAC Recommendations 1995)

Prepared for publication by

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Abstract

The calibration of high resolution infrared spectra is generally more precise than accurate. This is the case even when they are recorded with Fourier transform interferometers. The present note aims at improving the accuracy of wavenumber measurements in the infrared by recommending a selection of spectral lines as wavenumber standards for absolute calibration in the range from about 4 to about 7 000 cm⁻¹. Sources of frequency standards, on which the wavenumber determinations are based, are also given.

Introduction

The advent of high resolution Fourier transform interferometers has considerably improved the quality of the measurement of line profiles, and in particular the determination of their spectral positions. The wavenumbers of the rovibrational lines of the 2-O band of CO were proposed as standards in 73Gue with a derived value of the velocity of light, considered as a good check of the accuracy of these data. Additional checks, bringing additional confidence, were performed by comparing the positions of the lines of the 10 μm band 0001-[1000,0200]II of CO₂ measured by heterodyne techniques (74Pet) and by the same Fourier transform interferometer (82Gue). One year later heterodyne measurements were made on the 2-O band of CO (83 Pol), and Fourier spectra of the 10 μm band of CO₂ and of the 1-O band of CO (83Jen) were recorded. These two independent experiments revealed that the claimed accuracy of the previously given Fourier wavenumber standards was overestimated, and that they had to be slightly lowered. This was confirmed in 1985 by an extensive Fourier transform experiment (85Bro) where more details about these developments can be found.

These discrepancies between measurements from several sources have long been unexplained. This is one of the essential reasons why the present IUPAC working group "Unified Wavenumber Standards" was constituted in order to provide accurate wavenumber standards by combining complementary talents and tools to track the systematic errors. Extensive heterodyne frequency and Fourier wavenumber measurements have been performed. independent measurements of the same spectral features and critical comparisons of the various softwares used for their data processing have been realised. Also, the instrumental origins of the initial discrepancies are now better understood (90K ou).

Recommended heterodyne frequency standards.

The most accurate heterodyne frequency measurements are obtained with saturated absorption. In comparison, Doppler-limited lineshapes are generally measured with larger uncertainties. Our recommendations about the frequency standards to be used for calibration of infrared spectra are given in Tables 1 and 2, respectively for saturated absorption and for Doppler- limited frequency determinations. These two tables have a similar presentation. The two first columns give in the order of increasing lower spectral limit, the spectral limits $\tilde{\nu}$ in cm^{-1} , of the domain of the measurements. The third column reports the lowest and highest accuracies (in the form of estimated experimental uncertainties) of the measured line positions. Columns 4 and 5 respectively indicate which molecule² is concerned and in which publication the measured frequencies may be found³. Most often these papers provide also calculated frequencies which generally make a better coverage of the spectral range for calibration purposes than the experimental data. Almost all tables here refer however only to the measured transitions.

Figures 1 and 2 give a graphical representation of the spectral coverage of the data reported in Tables 1 and 2.

Recommended wavenumber standards

our recommendations are summarized in Table 3. The adopted presentation is the same as for Tables 1, 2, with an additional column reporting scaling factors⁴. Almost all⁵ toted references give extensive information. The recommended data have been generally determined using Fourier transform interferometers. A notable excepting is the book 91 Mak, which reports calculated wavenumbers derived from heterodyne frequency measurements.

¹Conversion from MHz to cm^{-1} is obtained by dividing by 29979.2458.

²In the column "Molecule", the isotopomers are not specified.

³The content of Tables 1 and 2 is not fully exhaustive. However, the data which have not been retained either have been remeasured by work reported in these tables, or are of no practical use for calibration purposes, as for instance those reported in 87Leo concerning the unstable NaH molecule.

⁴By virtue of Fourier transform interferometry, the offsets of the line positions given in the corresponding references, are corrected when multiplying the corresponding wavenumbers by this scaling factor.

⁵More precisely; 85Bro, 85Joh, 85Tot, 86Gue, 86Tot, 87Tot, 90Mor, 91Mak, 91 Tot1, 91 Tot2, 92Mor, 92Tot, 93Ger, 93Gue, 93Orm, 93 Tot 1, 93 Tot 2, 93 Tot3, 93 Tot4, 94Tot 1, 94Tot2, 94Tot3.

⁶Calculated frequencies of CO₂ corresponding to the CO₂ data cited in Table 1 may also be found in 91 Mak.

⁷The sc frequency measurements are cited in Tables 1 and 2.

Complete experimental spectral maps are provided in the three books 86Gue, 93Ger and 93Gue and in the two papers 90Mor, 92Mor. Extensive calculated spectral maps are also provided in the book 91 Mak. A selection of the best lines for calibration purposes is given in 91 Mak according to calculated uncertainties without evaluating possible overlappings. In the two books 86Gue and 93Gue a selection of the best transitions has been also performed. It is made according to the symmetry of the experimental profiles and its invariance with pressure-absorbing path conditions.

Figure 3 gives a graphical representation of the spectral coverage of the data reported in Table 3.

Conclusion

As shown from Figures 1, 2, 3 which summarise the content of Tables 1, 2, 3, the spectral range from 4 to about 5 000 cm⁻¹ is now provided with accurate standards. In contrast, in spite of some encouraging results (94deL), the near infrared range from 5 000 to 10 000 cm⁻¹ dramatically suffers from the lack of such high quality frequency measurements needed for the establishment of wavenumber standards.

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94Geo1	George, T., Urban, W., Le Floch A.: Improved Mass-Independent Dunham Parameters for the Ground State of CO and Calibration Frequencies for the Fundamental Band. J. Mol. Spectrosc. 16S (1994) 500-505.	
94Gc02	George, T., Wappelhorst, M. H., Saupe, S., Mürtz, M., W. Urban, W., Maki, A. G.: Sub-Doppler heterodyne frequency measurements of carbonyl sulfide transitions between 56 and 62 THz. J. Mol. Spectrosc. 167 (1994) 419-428.	
94Kou	Kou, Q., Guelachvili, G., Abbouti Tcksamani, M., Herman M.: The absorption spectrum of C ₂ H ₂ around $\nu_1 + \nu_3$: Energy standards in the 1.5 μ m region and vibrational clustering. Can. J. Phys. 72, 1241-1250, (1994)	
94Mak	Maki A. G., Chou C.-C., Evenson K. M., Zink L.R., Shy J.-T.: Improved molecular constants and frequencies for the CO ₂ laser from new high-J regular and hot-band frequency measurements. J. Mol. Spectrosc. 167 (1994)211-224.	
94 Mat	Matsushita, F., Evenson K. M., and Zink, L. R.: Absolute Frequency Measurement of Methanol form 1,5 to 6.5 THz. J. Mol. Spectrosc. 164 (1994) 517.	
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94Tot 1	Toth R. A.: The ν_2 and ν_3 bands of H ₂ ¹⁷ O and H ₂ ¹⁸ O: line positions and strengths. J. Mol. Spectrosc. 166(1994) 184-204.	
94Tot2	Toth, R. A.: Extensive Measurements of H ₂ ¹⁶ O Line Frequencies and Strengths - 5750 to 7965 cm ⁻¹ . Appl-Opt. 33:4851 (1994)	
94Tot3	Toth, R. A.: Transition Frequencies and Strengths of H ₂ ¹⁷ O and H ₂ ¹⁸ O from 6600 to 7640 cm ⁻¹ . Appl-Opt. 33:4868 (1994)	

Table 1
Saturated absorption heterodyne measurements

\tilde{v}_1 (cm ⁻¹)	\tilde{v}_2 (cm ⁻¹)	$d\tilde{v}^1$ (10 ⁻⁶ cm ⁻¹) (min. / max.)	Molecule	Reference
839.4	1106.6	1	CO ₂	80Fre ^c
849.2	907.2	3.5	CO ₂	81 Pet
851.4	1120.6	0.003/33	CO ₂	94Mak
896.5	944.2	0.5/6.7	CO ₂	84Pet ^a
903.2	1098.1	0.1/0.3	CO ₂	83Pet ^b
940.5	979.7	0.002/0.03	O ₃ 04	94Cha ^a
941.5	969.1	0.007/0.06	CO ₂	86Cha
942.4	942.4	0.1/0.5	SF ₆	82Bor ^b
942.4	951.0	0.17	SF ₆	87 Bob
944.2	951.2	0.1/0.5	SF ₆	83Bor ^b
946.0	946.0	0.1/0.5	SF ₆	79Bor ^b
1045.0	1070.5	3.3/33	OCS	90Fay
1686.7	1919.0	10	c o	89Sch2
1885.8	2064.6	0.7/1.6	o c s	94Geo2
2025.2	2111.5	0.2/2	c o	94Geo1 ^d
2082.0	2115.6	1.3/1.7	CO	91Wu ^a
2119.7	2119.7	1.7	CO	91Geo
2902.3	2909.4	1.7/2.5	Ocs	94Dax
2947.9	2947.9	0.1	CH ₄	80Kni
3693.4	3877.7	33	HF	91Goda
3698.0	3733.5	40	CO ₂	91Gro ^a
4180.3	4335.0	3	CO	83Pol ^b

^a The measurements given in this reference are also reported in 93Gue.

^b The measurements given in this reference are also reported in 86Gue.

^c This reference provides a wide range of calculated frequencies.

^d This reference 94Geo1 provides Dunham coefficients which may conveniently be used to calculate a wide range of CO line positions.

¹ The absolute uncertainty of the measurements is $\pm \tilde{d}\tilde{v}$.

Table 2
Doppler-limited heterodyne measurements

$\tilde{\nu}_1$ (cm ⁻¹)	$\tilde{\nu}_2$ (cm ⁻¹)	$d\tilde{\nu}^2$ (10 ⁻³ cm ⁻¹) (min. / max.)	Molecule	Reference
3.8	144.8	0.03/1.5	CO	92Var ^a
20.9	206.7	3.5/13	HCl	87Nola ^a
22.1	109.7	1.7/3.5	CO	90Zin ^a
26.3	37.6	6.7	OCS	89 Van2a
41.1	204.5	7/44	HF	87Jen, 87Nola ^a
41.7	206.4	3.5/1.3	HCl	87Nola ^a
49.6	216.4	0.00033/0.012	CH ₃ OH	94Mat ^a
50.1	50.2	6.7	N ₂ O	89Van2a
853.7	886.0	0.066/0.2	Ocs	81Wel1a
858.6	889.8	0.070/0.2	Ocs	81 Wel2a
888.5	959.4	0.02/0.35	CO ₂	84Pet ^b
896.9	989.7	0.1/0.35	N ₂ O	89Mak ^b
956.2	1086.0	0.27	HF	88Jen ^a
1031.5	1035.5	0.070	Ocs	79Wel ^b
1037.2	1084.6	0.13/0.27	N ₂ O	87Zin ^b
1046.8	1090.5	0.10	Ocs	81Sat2
1056.6	1087.7	0.10	Ocs	90Fay ^a
1068.9	1085.9	0.20	SO ₂	81Sat1
1104.8	1109.8	0.2/0.5	N ₂ O	85Wel2a
1257.1	1931.4	0.10	CO	89Sch2 ^a
1257.3	1339.8	0.07/0.33	N ₂ O	85Wel1b
1257.4	1335.0	0.067/0.35	N ₂ O	87Hin ^b
1349.5	1394.2	0.1/0.5	SO ₂	90Van ^b
1363.6	1397.4	0.17/1.2	Ocs	89Sch1b
1462.9	1549.0	0.07/0.25	CS ₂	88Wel ^b
1591.3	1672.7	0.17/0.35	N ₂ O	89Van1b
1641.2	1961.8	0.2/0.6	HBr	84Wela ^a
1650.8	1736.7	0.1/1	Ocs	89Wel ^b
1686.7	1725.3	0.1/0.67	Ocs	83Wela ^a
1750.1	1931.7	0.133/0.33	NO	86Hin ^b
1834.7	1914.7	0.17/0.5	N ₂ O	85Wel2a
1850.8	1914.6	0.2/1.35	Ocs	88Mak ^b

²The absolute uncertainty of the measurements is $\pm \delta\nu$.

1866.8	1914.9	0.133/0.33	OCS	86Mak ^a
1991.2	2085.4	0.1/0.5	OCS	90Wel ^b
1995.1	2068.8	0.1/0.17	CO	90Sch ^b
2008.3	2081.3	0.1/0.5	CO	90Mak ^b
2100.9	2138.1	0.1/0.5	OCS	90Mak
2898.6	2912.8	0.17/0.3	OCS	92Dax ^b
4120.7	4350.7	0.27/0.67	CO	83Pol ^a
4341.1	4753.3	0.13/0.4	N ₂ O	84Pol ^a
6563.3	6564.4	0.9/2.2	NH ₃	91Sas ^b
6563.3	6563.3	0.9/1.1	HCN	91Sas ^b
6563.4	6564.5	1/1.2	H ₂ O	91Sas ^b
6563.4	6564.5	1.2	C ₂ H ₂	91Sas ^b

The measurements given in this reference are also reported in 86Guc.

^b The measurements given in this reference are also reported in 93Guc.

Table 3
Recommended wavenumber standards

$\tilde{\nu}_1$ (cm ⁻¹)	$\tilde{\nu}_2$ (cm ⁻¹)	Scaling ³ Factor	$d\tilde{\nu}^4$ (10 ⁻³ cm ⁻¹) (min. /max.)	Molecule	Reference
25	350		0.2/0.5	H ₂ O	85Joh, 86Gue
100	200		0.05/0.5	CH ₃ OH	90Mor
200	350		0.5	CH ₃ OH	92Mor
205	1086		0.2/2.5	HF	87Jen
354	1447		0.03/0.4	H ₂	83Jen
486	567	1.0	0.15/0.18	Ocs	91Mak
501	713		0.2/0.5	H ₂ O	86Gue
523	659		0.08/0.22	N ₂ O	91Mak
543	636	1.000000320	0.2/0.5	N ₂ O	86Gue
719	1194		0.2	NH ₃	86Gue
812	890	1.000000035	0.05/0.28	Ocs	91Mak
814	1116		0.1	NH ₃	85Bro
823	889	1.000000070	0.2/0.5	Ocs	86Gue
880	1087		0.001/0.09	N ₂ O	91Mak
900	1090		0.05/0.3	N ₂ O	87 Tot
900	4700		0.05/0.3	N ₂ O	91 Tot2
913	1573		0.06	H ₂ O	93Tot4
924	1090		0.1	CO ₂	85Bro
969	1891		0.06	H ₂ O	93Tot3
1000	1095	1.0	0.011/0.13	Ocs	91Mak
1009	2224		0.06	H ₂ O	92Tot
1022	1077		0.02	Ocs	92Hor
1206	2095	0.999999770	0.5	H ₂ O	86Gue
1066	2582		0.06	H ₂ O	91Tot1
1100	1440		0.06/0.3	N ₂ O	86Tot
1105	1345		0.05/0.28	N ₂ O	91Mak
1118	1250	(0.999 997273 + 0.0031 $\tilde{\nu}$)	0.5	N ₂ O	86Gue
1132	1329		0.1	N ₂ O	85Bro

³See text The absolute uncertainty $\tilde{d}\tilde{\nu}$ in column 4 of the table does not take into account the improvement in quality brought by this scaling factor 011 the corresponding measurements.

⁴The absolute uncertainty of the measurements is $\pm \tilde{d}\tilde{\nu}$.

1200	1430		0.1	CO ₂	85 Tot
1218	1380		0.1	CH ₄	89Cha
1250	1343	0.999999761	0.5	N ₂ O	86Gue
1304	1934		0.06	H ₂ O	93 Tot 1
1309	1594	0.999999717	1	CH ₃ Cl	93Gue
1339	1992		0.1	H ₂ O	85Bro
1460	1551		0.08/0.23	CS ₂	91Mak
1580	2380		0.05/0.3	N ₂ O	87Tot
1650	1739	1.000000005	0.08/0.34	Ocs	91Mak
1741	1940	0.999999980	0.21/0.40	NO	91 Mak
1780	1952		0.05	NO	94Spe
1820	1925		0.0-//0. 14	N ₂ O	91Mak
1820	2571		0.06	H ₂ O	93Tot2
1831	2830	0.999999764	1	N ₂ O	86Gue
1832	1934	0.999999983	0.09/0.28	Ocs	91Mak
1948	2275		0.003/0.08	c o	91Mak
1963	2059		0.05	Ocs	92Mas
1970	2141	1,000000015	0.09/0.25	Ocs	91Mak
2086	3162		0.2	HC1	93Rin
2140	2269		0.05/0.08	N ₂ O	91Mak
2234	2391	0.999999 8] 7	1	CO ₂	86Gue
2350	23600		1	Fe J. Fe II	92Nav
2400	2607		0.07/0.32	N ₂ O	91 Mak
2510	2600		0.1 ?./0.33	Ocs	91Mak
2630	2774	0.999999817	1	C ₂ H ₂	93Gue
2622	4260		0.06	H ₂ O	93Tot 1
2693	2763	1.000000024	0.24/0.88	Ocs	91Mak
2700	2760	0.999999795	1	Ocs	93Gue
2725	2842		0.09/0.22	N ₂ O	91Mak
2820	3119	0.999999811	1	Ocs	93Gue
2862	2970	1.0	0.1 6/0.21	Ocs	91Mak
2912	4506		0.06	H ₂ O	93Tot2
2925	3000		1	C ₂ H ₄	86Gue
2947	2947		0.1	CH ₄	85Bro
3001	3648	0.999999789	1	NH ₃	93Gue
3001	4340		0406	H ₂ O	94 Tot 1
3065	3120	1.0	0.3/0.9	Ocs	91Mak
3665	3831	0.999999929	1	CH ₃ Cl	93Gue
3797	4134		0.2/0.5	CH ₄	88Bro
3801	3976	0.999999754	1	C ₂ H ₂	93Gue
3849	4001	0.999999917	1	CH ₃ I	93Gue
3996	4170	0.999999884	1	C ₂ H ₂	93Gue
4071	4352		0.00?/0.11	c o	91Mak
4080	4340	0.999999917	1	NH ₃	93Gue

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4300	4653	0.999999917		1	NH ₃	93Gue
4328	4755	0.999999924		1	N ₂ O	93Gue
4381	4749		0.1		N ₂ O	85Bro
4781	4870	0.999999917		1	CH ₃ I	93Gue
4820	5234	0.999999917		1	NH ₃	93Gue
4879	5130	0.999999917		1	N ₂ O	93Gue
5103	5548	0.999999917		1	H ₂ O	93Gue
5341	5825	0.999999891		1	HCl	76Gue
5668	5992	0.999999914		1	CH ₃ I	93Gue
5750	7987		0.5/1		H ₂ O	94Tot2
5956	6237	0.999999907		1	CH ₃ I	93Gue
6030	6880		0.2		H ₂ O	93Orm
6373	6611		0.2		H ₂ O	94B yk
6378	6395		0.5		HCN	90Sas
6385	6388		2		c o	92Yos
6432	6683		0.3		C ₂ H ₂	94Kou
6450	6685	0.999999916		1	C ₂ H ₂	93Gue
6607	7639		0.1/1		H ₂ O	94Tot3
7220	11200		5		I ₂	93Ger
7277	7997	0.999999942		1.5	HF	76Gue
		

Figure Caption.

Figure 1: Spectral coverage of the data given in ‘l’able 1. Spectral ranges are sequentially displayed above each other according to their lower spectral limit, in the same order as in the corresponding table.

Figure 2: Spectral coverage of the data given in Table 2. Spectral ranges are sequentially displayed above each other according to their lower spectral limit, in the same order as in the corresponding table.

Figure 3: Spectral coverage of the data given in Table 3. Spectral ranges are sequentially displayed above each other according to their lower spectral limit, in the same order as in the corresponding table.

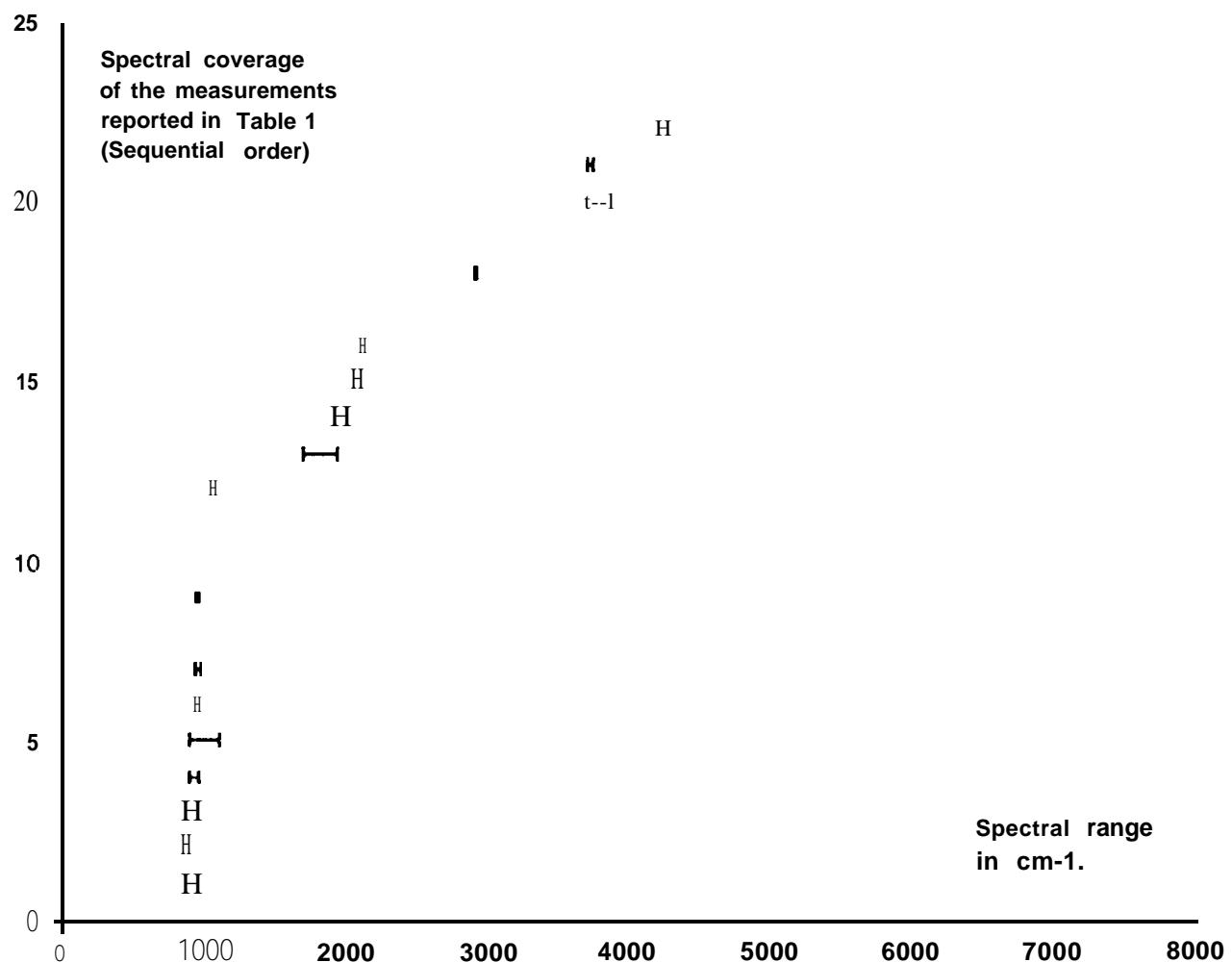


Figure 1: Saturated absorption heterodyne measurements

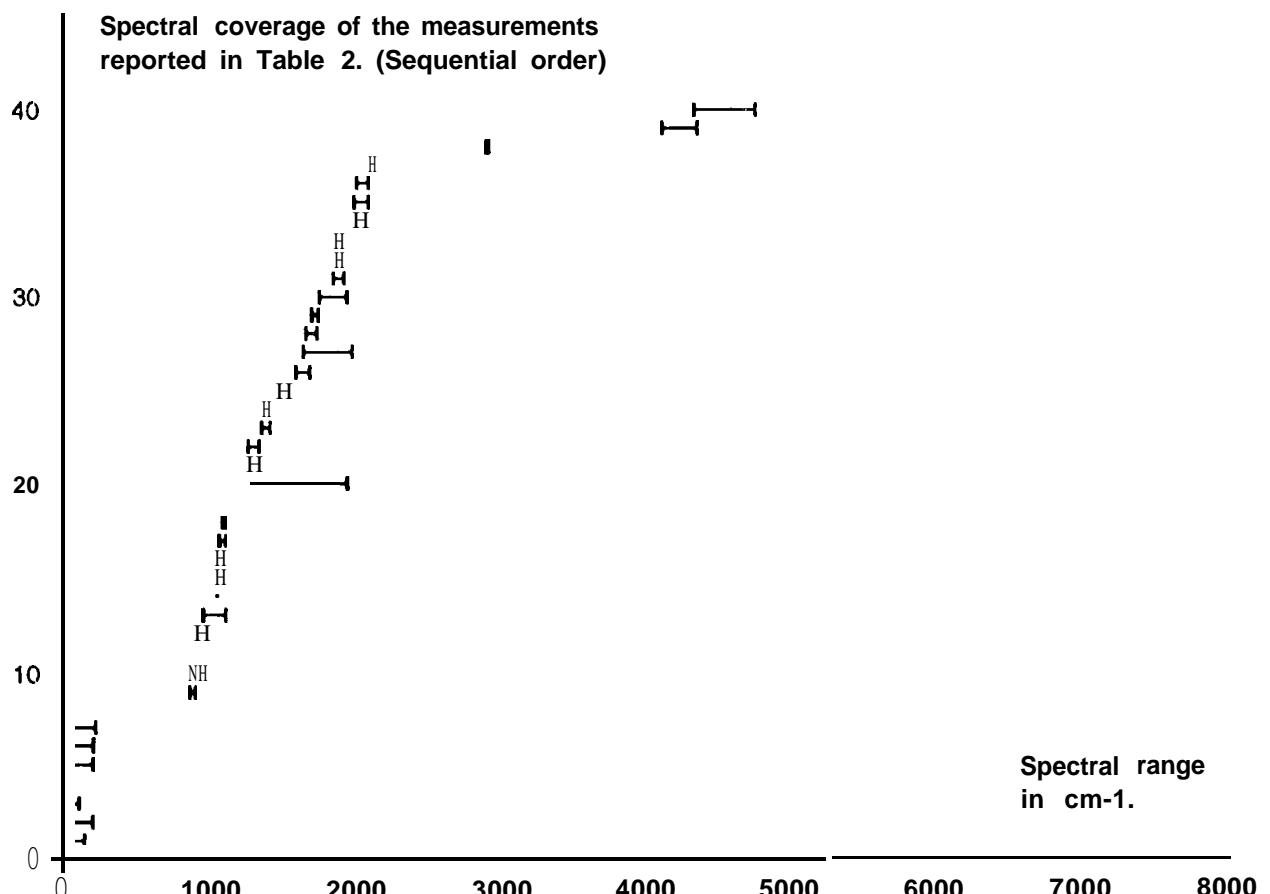


Figure 2: Doppler-limited heterodyne measurements

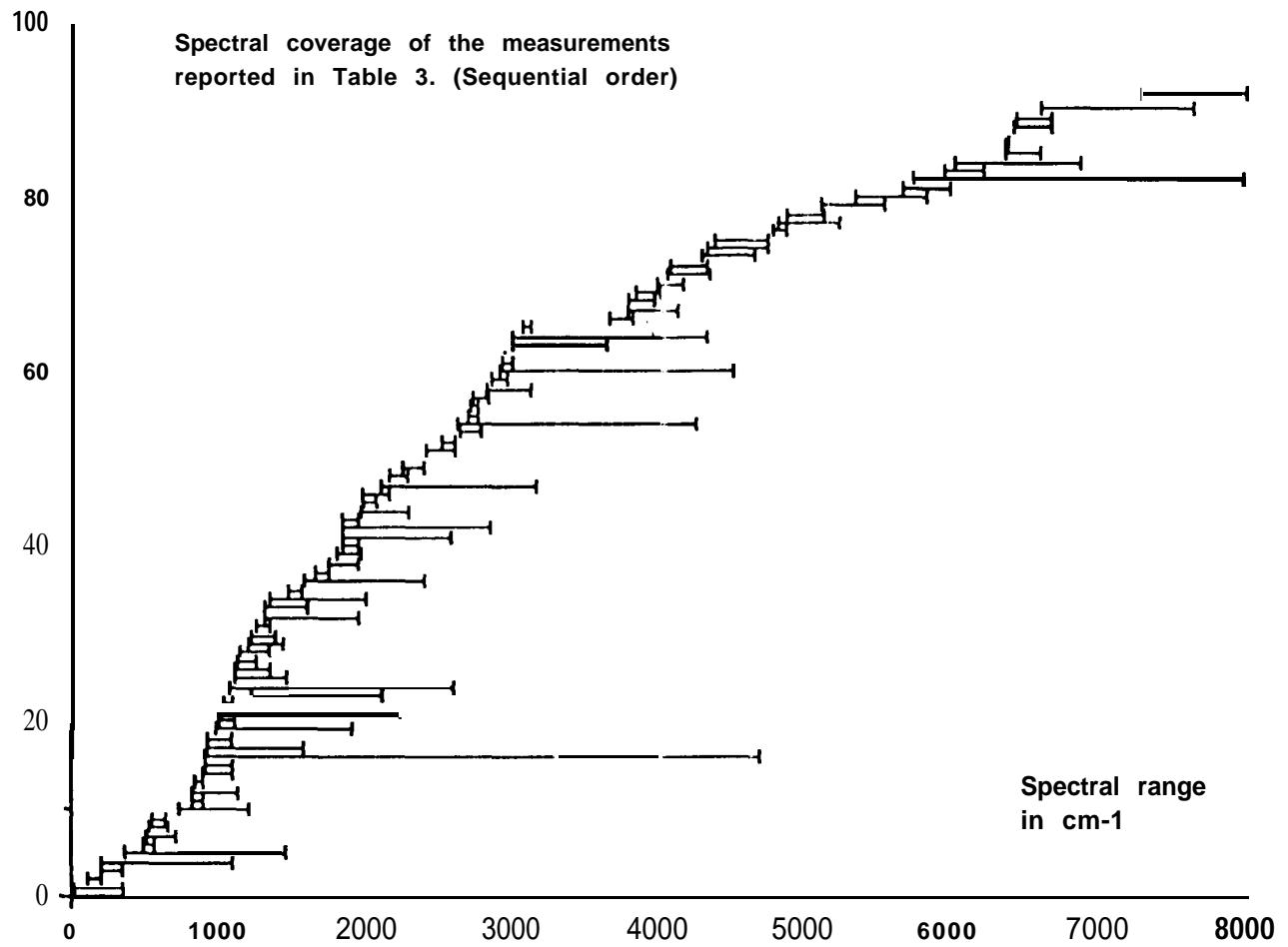


Figure 3: Recommended wavenumber standards